

Transient Evolution of a Planar Diffusion Flame Aft of a Translating Flat Plate

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ABSTRACT

The high degree of spatial symmetry of a planar diffusion flame affords great simplifications for experimental and modeling studies of gaseous fuel combustion. Particularly, in a microgravity environment, where buoyancy effects are negligible, an effectively strain-rate-free, vigorous flame may be obtained. Such a flame can also provide long residence times and large length scales for practical probing of flame structures and soot processes. This 2-D numerical study explores the feasibility of establishing such a planar diffusion flame in an enclosed container utilizing a realistic test protocol for a microgravity experiment. Fuel and oxygen mixtures, initially segregated into two half-volumes of a squat rectangular container by a thin separator, are ignited as soon as a flammable mixture is formed in the wake of the separator withdrawn in the centerplane. A triple-flame ensues that propagates behind the trailing edge of the separator. The results of calculations show that the mechanically- and thermally-induced convection decays in about two seconds. The establishment of a planar diffusion flame after this period seems feasible in the central region of the container with sufficient quantities of reactants left over for subsequent studies. An analysis of the flame initiation and formation process suggests how the feasibility of creating such a flame can be further improved.

INTRODUCTION

A numerical model is developed to check the feasibility of creating a virtually strain-rate-free, planar diffusion flame in an enclosure under buoyancy-free environments. This study is inspired by the original concept of Fendell, F., *et. al.* [1–5] for a microgravity experiment which lends itself to simplified 1-D mathematical analysis, owing to its high degree of spatial symmetry. Such a flame constitutes the most vigorous laminar burning [6] and also provides long residence times and large length scales to facilitate detailed diagnostic probing of flame structures and soot/particle formation processes. The conceptual design involves a squat rectangular container which is divided by a separator at the centerplane (mid-height) into two equal half-volumes. Initially, one half-volume is filled, for example, with hydrogen, diluted with argon, and the other half-volume is filled with oxygen, diluted with helium, such that the temperature, pressure and density in the two half-volumes are equal. Ideally, the separator between the segregated reactants is to be “eliminated”, and the thin layer of combustible mixture, resulting from a brief interval of interpenetration of reactants, is to be ignited uniformly at the centerplane. In the absence of buoyancy, a diffusion flame is expected to be formed and should remain planar. Such a flame in earth gravity would be disrupted in less than a second owing to Rayleigh-Benard instability [7].

Numerical studies of combustion in enclosures are challenging due to the large range of time scales arising in low-speed, compressible, exothermic flows. There is need to account accurately for the effect of acoustic waves on the compressible pressure field. A time step sufficiently small for accurate temporal resolution, yet large enough to avoid numerical truncation error build-up, has been determined by using a 2-D numerical code [8] to compute a special scenario with known 1-D solution. In more detail, adoption of idealized slippery, adiabatic and non-reacting/non-catalytic sidewall boundary conditions admits a 1-D solution, provided the initial conditions are appropriately chosen. Indeed, the time-step sizes, which permit recovery of the known 1-D solution, are consistent with the characteristic acoustic, chemical reaction and diffusion time scales for the conceptual experiment in the idealized enclosure. Improper choices of the time-step size result in miscalculation of the adjustment of the flow to the heat-release rates, and in particular, to inaccurate local pressure fields. Next, the 2-D model addressed more realistic no-slip, cold and non-reacting/non-catalytic sidewall boundary conditions, but again for idealized uniform ignition at the undisturbed fuel/oxidizer interface. The calculations predict a planar diffusion flame, except for quenching near the cold sidewalls, and convection generated due to thermal expansion decays in less than a second. Thus, creating a virtually strain-rate-free, planar, (in general) traveling diffusion flame in a suitably configured container is predicted to be possible in these idealized cases.

The study presented here focuses on generating such a flame in a physically realizable container *under a realistic separator-removal and ignition scenario*. In this scenario [9], the separator is a thin metallic plate which is removed, by lateral translation in its own plane, through a tightly-fitting slit in one sidewall. Ignition by spark is to occur along a line (point for 2-D) near and parallel to the sidewall from which the trailing edge of the separator departs when the separator begins to translate. The ignition spawns a triple-flame which propagates through a thin layer of interdiffused reactants, and which propagates in the direction of separator motion. Whether the convection generated by the separator-entrained gases, thermal expansion, and triple-flame propagation decays sufficiently quickly for a planar diffusion flame to develop in the centerplane is explored.

DESCRIPTION OF THE MODEL

An experimental container fabricated for testing is 25cm long x 25cm wide x 9cm high with impervious, isothermal, non-catalytic walls. A 0.9mm-thick metallic separator divides the container into two half-volumes, each 4.5cm high. The solid surfaces are kept at 298K, and the gases are initially at 298K and 1atm.

A transient, 2-D (25cm long x 9cm high) computational study of this system accommodates the temporally evolving, but effectively spatially uniform, rise of pressure in the enclosure under one-step irreversible hydrogen-oxygen chemistry. The thermodynamic and transport properties of the gas mixture are chosen to be consistent with NASA CET [10] predictions for the *equilibrium mixture* obtained under *adiabatic* conditions, and the binary diffusion coefficient of each species with the mixture is adopted. The temperature dependence of properties is approximated by power-law fits. The code calculates the density field based on the temperature, pressure and average

molecular weight of the mixture. The pressure dependence of the binary diffusion coefficients is also accounted for by discrete readjustments of code-input values whenever pressure varies by 10%. An Arrhenius rate expression for the global chemical reaction is available [11].

The translation speed of the separator is taken to be uniform at 1m/s in this study. This speed is intermediate, between slower speeds that incur larger lateral nonuniformities in what is intended to be a planar flame experiment and larger speeds that allow faster diffusion-flame emplacement but may incur instabilities and transition to turbulent flow. The continuous separator motion is conveniently modeled by a sequence of instantaneous, discrete translations, between which a *moving*, but no-slip, boundary condition holds on the portion of separator surface remaining within the container. Thus, the calculations are stopped every 10ms, during which a continuously moving separator would have traveled a distance of 1cm; a 1cm-long piece of the trailing edge of the separator is deleted and replaced with fresh quiescent gases before restarting the calculations. Hence, the separator is advanced across the 25cm-long container in 25 discrete steps. Gas is introduced such that the contact interface of initially separated gas mixtures is at the half-height of the separator thickness with no thickness, (*i.e.*, without interpenetration). Thus, one half of each deleted solid segment is filled by a 1cm-long x 0.45mm-high segment of the initial hydrogen/argon mixture, and the oxygen/helium mixture fills the other half. This fresh gas addition to the container is modest because the separator thickness is only 1% of the container height. Since the trailing end of the experimental separator is tapered to a sharp edge, rather than being left blunt, this numerical description should be more representative than taking a premixture to fill the truncated separator segment.

The time-step size of 10 μ s provides sufficient temporal resolution, as discussed earlier. For sufficient spatial resolution, 200 uniformly distributed and 70 uniformly graded cells are used to span the length and height of the container, respectively. Thus, the resolution along the length is uniform at 125mm. Two 0.45mm-high cells define the separator thickness, the minimum resolution in the height coordinate. The grading along the height is such that the heights of two adjacent cells do not differ by more than 20%, and such that the aspect ratio of every cell is between 0.125 and 8, to provide adequate numerical stability. Sufficient spatial resolution is confirmed for ideal, lengthwise-uniform-ignition scenarios by comparing the results obtained from uniformly distributed grids of 200 x 70 and 100 x 36. The computed maximum values of velocity, temperature and reaction rate differed by less than 4% from one another at all times up to 0.5 seconds.

Ignition is numerically simulated by assigning an initial temperature of 1500K to the cells covering a small area of about 5mm x 1mm, at a distance of about 7mm from the sidewall and 1mm above the separator. The size and position of these cells are representative of the experimental spark igniter. Ignition is triggered 10 μ s (numerical temporal resolution) after the trailing edge of the separator is shifted by 1cm to a position 2cm away from the sidewall, thereby clearing the igniter location (see Fig. 1). Figure 1 shows that the maximum temperature is 1540K, which indicates a rise of 40K during the first 10 μ s, a time interval too short for appreciable thermal diffusion. Pressure waves, on the other hand, are moving at sonic speeds and are carefully accounted for during ignition by sufficient temporal resolution for correct simulations of the resultant flow field.

However, the fast travel of the acoustic waves in the container via wall reflections and their small amplitude allow pressure to be considered effectively spatially uniform, for most purposes.

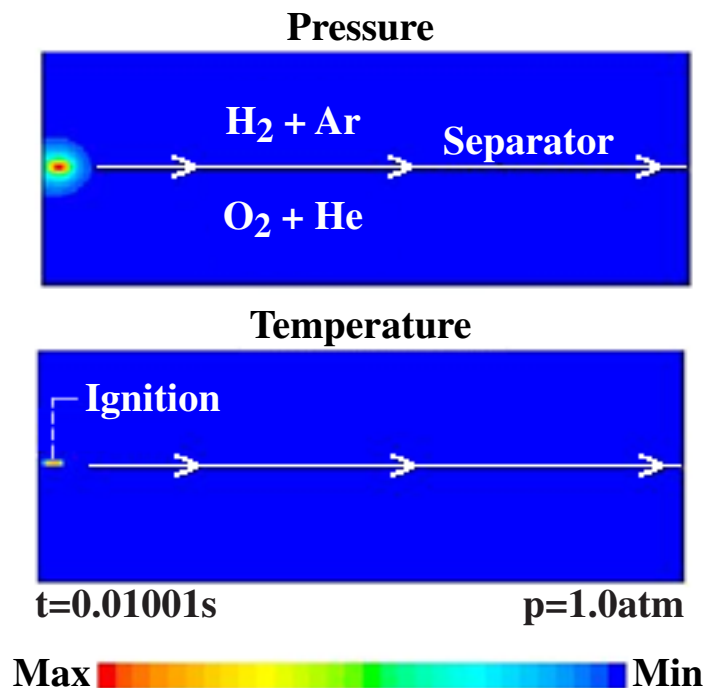


Figure 1 – Flame ignition. Pressure and temperature fields 10 μ s after “spark” at 1500K. $T_{\max}=1540$ K. The same linear scale applies to all subsequent Figures.

This study is a simulation of overall-hydrogen-deficient burning, chosen to constrain thermal-expansion-induced convection. However, vigorous combustion is still desired at early times before extinction occurs due to reactant depletion and/or heat loss. The initial reactant concentrations correspond to a hydrogen/oxygen equivalence ratio of 0.2, if the contents of the half volumes were to be mixed homogeneously. Hence, the initially premixed species mass fractions in the container would be $[H_2]=0.0122$, $[Ar]=0.4878$, $[He]=0.0122$, and $[O_2]=0.4878$ (on a molar fraction basis: $[H_2]=0.1667$, $[Ar]=0.3333$, $[He]=0.0832$, and $[O_2]=0.4168$). In the scenario of interest, H_2 and Ar occupy initially only one half-volume, and O_2 and He occupy the other half-volume. The adiabatic flame temperatures, using the NASA CET code [10] for the premixed gases initially at 298K and 1atm, are 1774K for constant pressure, and 2234K for constant volume. The computed final pressure of the constant volume burn is 6.8atm. Although the diffusion flame burning in the experiment takes place in a constant-volume container, the time scale for the diffusion-constrained combustion is such that the rate of pressure rise or decay is governed by heat loss. Thus, the combustion occurs effectively at a succession of pressures, and hence, the adiabatic flame temperature at constant pressure is also informative.

DISCUSSION OF RESULTS

The results are discussed for two separate time periods within the interval of numerical integration, which continued to 2 seconds (chosen as a typical duration for a microgravity experiment conducted at the 2.2-second drop tower facility at NASA Glenn Research Center). The first period is referred to as the flame-initiation period during which ignition occurs at a point near one sidewall, and a thin flame propagates aft of the separator's wake, with the flame reaching the other sidewall after the trailing edge of the separator exits the container. The second period is referred to as the flame-formation period, during which the convection generated in the container decays and a diffusion flame with planarity is approached.

During the flame-initiation period, there are two sources for generating convection in the container: one imparted by the continuous withdrawal of the separator, and another created by the flame-induced gas expansion. Since the separator-removal speed is taken as 1m/s, it takes 0.25s for the separator to leave the 25cm-long container. Figure 2a shows the flow and temperature fields 0.1s after the separator is set into motion. The gases entrained by the separator, but not permitted to exit the container, return toward the center of the container from the exit sidewall in each half volume. The return drift is slow relative to the separator-entrained flow in the narrow layer near the centerplane due to the broader return area available, and would be even slower for larger half-heights of the container. Similarly, the thermal expansion of burned gases from the flame deflagration creates an appreciable flow directed, this time, toward the sidewall with the igniter which, in turn, generates return flows opposite in motion to the separator-induced ones in each half volume. The nature of the flame propagation, which results from igniting the stratified combustible mixture formed by the interpenetration of reactants aft of the separator, is described as a triple-flame. The temperature field indicates that the tip of the triple-flame lags behind the trailing edge of the separator. Although no one single speed fully describes the triple-flame, its propagation speed can be characterized by the maximum speed pertaining to the near-stoichiometric mixture in our single-step model. In our numerical studies, the flame propagation speed for a simplified case in which the separator is absent is slower ($\sim 0.6\text{m/s}$) than the separator withdrawal speed of 1m/s used in this study. The bifurcating and returning flow enhances the thickening of the hot zone near the sidewall. The pressure rises by 0.1atm during the first 0.09s after ignition.

Figure 2b shows the flow and temperature fields 0.2s after the separator is set into motion, so 80% of the separator has exited the container. The flow field reveals two compensatory return flows, one from each sidewall, in each half volume. Thermal expansion of gases leads to flows both in the horizontal and vertical directions. The strength and resultant direction of these flows depend on the instantaneous position of the propagating triple-flame. Besides the gases entrained by the separator's surface, further gases are entrained into the wake flow aft of the trailing edge of the withdrawing separator. The nearly unchanged gap between the trailing edge of the separator and the tip of the triple-flame in Figs. 2a and 2b indicates that the otherwise slower flame ($\sim 0.6\text{m/s}$) has caught up with the trailing "edge" of the wake flow. Thus, the flame propagation speed is now the sum of the wake-flow speed plus the flame propagation speed. However, the flame tip can not get closer to the trailing edge of the separator than the distance necessary to form a combustible mixture (since the cold separator surface does not appear to be the cause of quenching). Near the sidewall, convective flow thickens the warm-gas zone beyond what is ascribable to diffusion alone.

Further combustion in this region lets temperatures exceed the (premixture) adiabatic flame temperatures. The increasing burning area leads to an enhanced rate of pressure rise.

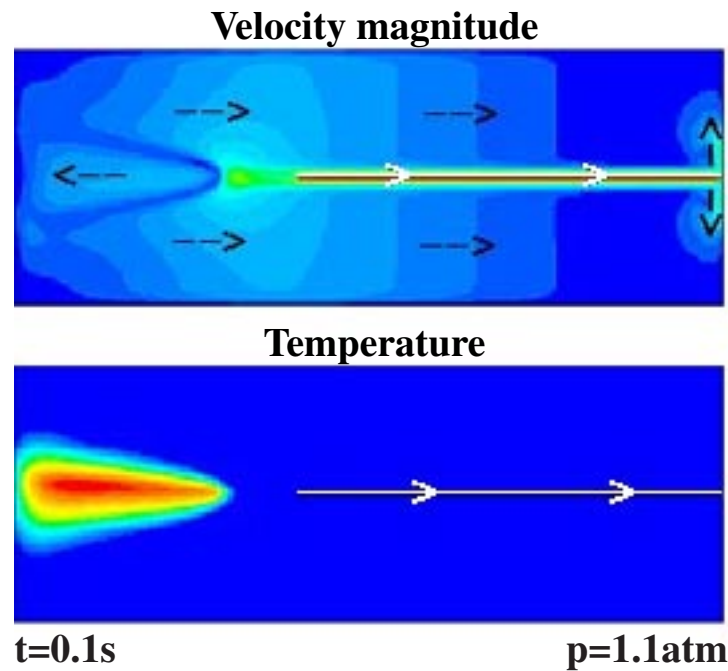


Figure 2a – Flame initiation. Velocity and temperature fields 0.1s after separator starts moving at 1m/s. $V_{\max}=1\text{m/s}$, $T_{\max}=2182\text{K}$.

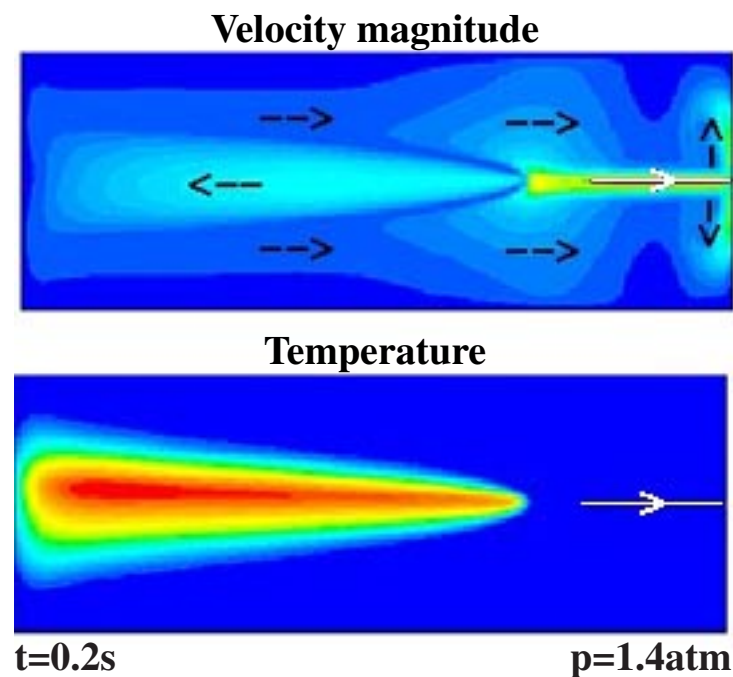


Figure 2b – Flame initiation. Velocity and temperature fields 0.2s after separator starts moving at 1m/s. $V_{\max}=1\text{m/s}$, $T_{\max}=2383\text{K}$.

Figure 2c depicts the conditions 0.03s after the separator exits the container. The flow field shows the formation of two small recirculations confined in the vicinity of the exit sidewall, one in each half volume. The separator-entrained gases, which are not permitted to exit the container, split toward the top and bottom corners and reach substantial speeds. The broad return-flow recirculations, created by separator withdrawal and burned gas expansion, form an organized flow pattern which enhances the diffusional transport toward the centerplane. Until this flow pattern decays, it modifies the rate of burning in the container. The temperature continues to rise at the ignition end of the flame, despite the increasing heat loss to the cold sidewall and decreasing reaction rate, as indicated by the production rate of water. During the initiation period, the location of maximum temperature is not related to the instantaneous location of maximum reaction rate; *i.e.*, combustion may be faster in cooler regions. This suggests that special care must be given to the interpretation of experimental data. The reaction rate demonstrates that a nearly flat flame is established. The flame has slightly traveled into the leaner hydrogen side and is weaker in the broader warm-temperature region. The reaction rate is not only stronger in the thinner region but is further enhanced by the fresh reactants delivered by the counter-rotating vortices. The pressure rise accelerates, despite higher heat loss to container walls, due to the increased flame area and convective contribution to conversion of reactants per area of flame. The upshot after the initiation period is that the established flame is planar, but it is not uniform, and transport is not primarily controlled by diffusion yet.

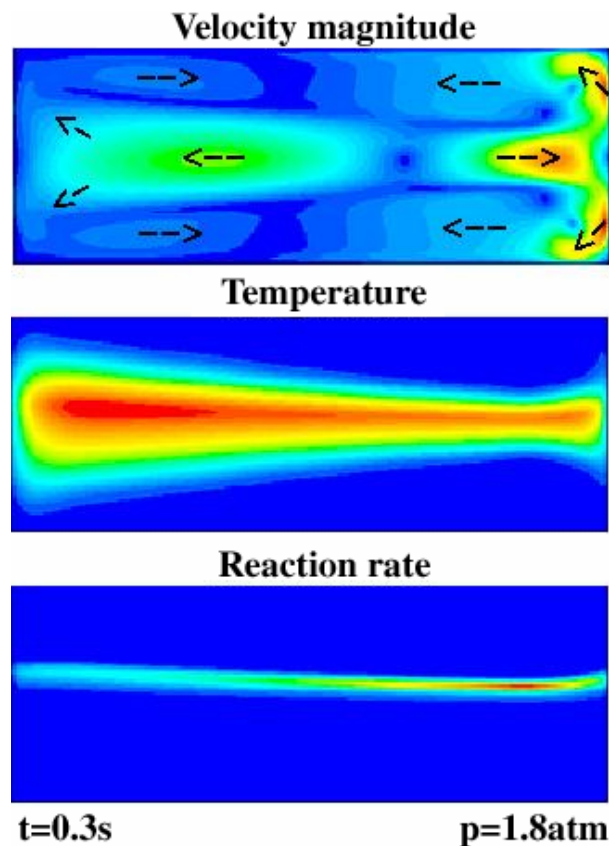


Figure 2c – Flame initiation. Velocity, temperature, and water production rate fields 0.3s after separator starts moving at 1m/s. $V_{max}=0.36m/s$, $T_{max}=2487K$, $RR_{max}=2.2Kg/m^3/s$.

Diffusionally-dominated transport starts when the convection generated during flame initiation decays appreciably via viscous dissipation, as shown in Fig. 3a. The maximum gas velocity 0.75s after the separator leaves the container is $\sim 10\%$ of that of the separator withdrawal. The vortices near the exit sidewall have moved slightly toward the center of the container and have enhanced the depletion of reactants near the sidewall, as evidenced by the flame position, which has shifted toward the (stoichiometrically-deficient) hydrogen side. The larger return-flow recirculations occupy four roughly-equal quadrants of the container, and continue to decay. The temperature field reflects the resultant cumulative effects of convection and suggests that the remaining reactants are displaced from the sides toward the center of the container. The nonuniformity of the flame persists, though the flame remains relatively flat. The rate of temperature rise has slowed considerably due to slower combustion and increasing rate of heat loss. The container pressure has reached 3atm.

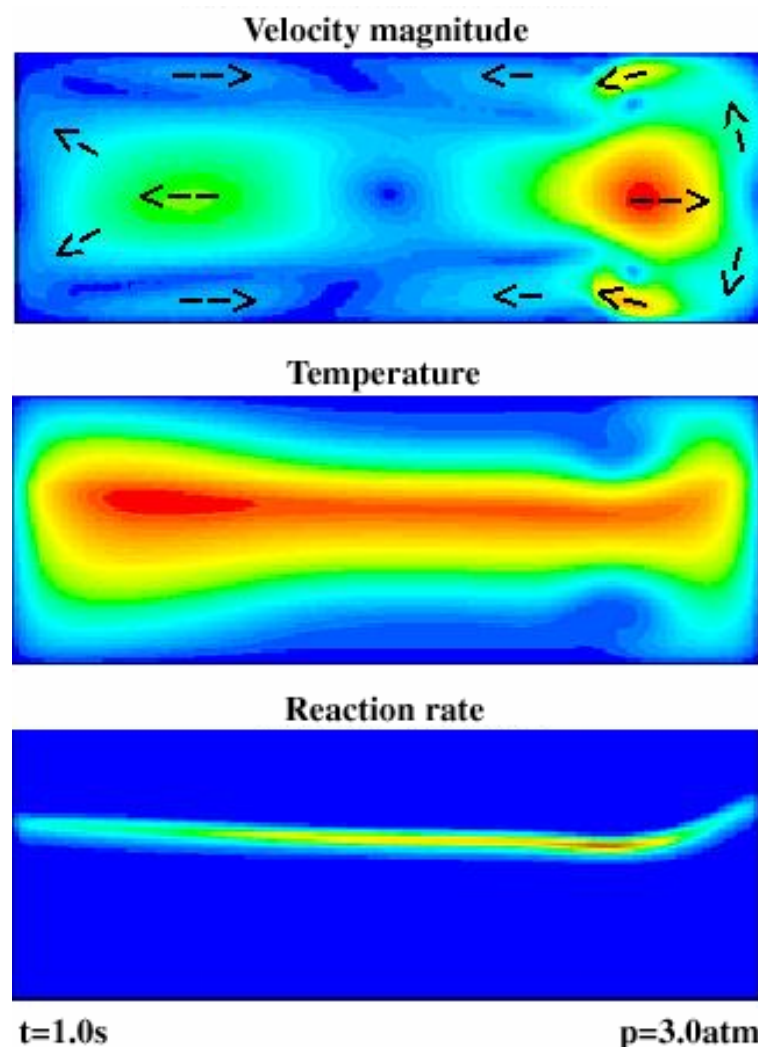


Figure 3a – Flame formation. Velocity, temperature, and water production rate fields 1.0s after separator starts moving at 1m/s. $V_{\max} = 0.10\text{m/s}$, $T_{\max} = 2561\text{K}$, $RR_{\max} = 1.2\text{Kg/m}^3/\text{s}$.

A snapshot of the conditions in the container 2 seconds after the separator's motion is shown in Fig. 3b. Velocities have diminished to levels at which transport is not dominated by convection anymore, especially for fast-diffusing hydrogen. The expected conduction-governed temperature profile is almost established between the top and bottom walls, and there is increased heat loss to these walls. Since the reaction rate has also further slowed, the maximum temperature of the flame has started to decrease. The growth of the sidewall quench layers is evident and the maximum temperature displays a planar uniformity in the core of the container. The reaction rate profile indicates that a relatively flat, uniform, and about 10cm-wide flame, which is increasingly diffusion-dominated as time passes, is established in the core of the container. In fact, the flame has slightly traveled toward the hydrogen half-volume. The temperature and both hydrogen and oxygen concentration profiles are consistent with these observations. With the described flow in the container, and without account for condensation, the accumulation of water vapor near the sidewalls is evident. The pressure in the container is 3.9atm and continues to climb. The maximum hydrogen mass fraction is 0.0215, which is quite high relative to its initial value of 0.0244. The hydrogen that remains is concentrated in a colder region near the top wall, and has a relatively high density, so a substantial quantity of the stoichiometrically deficient reactant hydrogen is left to sustain combustion. Richer initial hydrogen concentrations, up to stoichiometrically-balanced quantities of hydrogen and oxygen, would result in reduced diffusional-flame travel, and more leftover hydrogen implies longer time until extinction. The stoichiometrically-balanced diffusion flame would hover mostly near the centerplane.

Creating a planar diffusion flame, which accommodates a convenient 1-D analysis, is feasible in this container, under the described flame initiation scenario for buoyancy-free conditions. The growing sidewall quench layers, as well as reactant transport in the horizontal direction, might eventually disallow a 1-D treatment of the combustion phenomenon in the core of the container by intruding on the width of the uniform portion of the planar flame. This also suggests that the selection of the area for focusing the experimental diagnostics is critical. Improvements to the container design and experimental procedure for increased feasibility are possible [1]. Further numerical studies are currently underway toward that end, including the effects of separator-translation speed, ignition delay time, and addition of baffles/screens into the container. Increasing the height of the container would reduce the speed convection and increase reactant availability for longer-duration diffusion-flame experiments, provided Rayleigh-Benard instabilities are not introduced for the level and quality of microgravity available for space experiments. Furthermore, since hydrogen diffuses much faster than gaseous hydrocarbon fuels, and since the heat-release rate of diffusion-controlled hydrogen-oxygen reaction is larger than for hydrocarbon burning, the scenario considered in this study is a conservative (stringent) test of feasibility.

SUMMARY AND CONCLUDING REMARKS

This paper addresses whether a new experimental apparatus proposed for creating a planar, virtually strain-rate-free diffusion flame in microgravity would "work" in accord with its design. If successful, then an entire new class of experiments on vigorous non-premixed burning, inaccessible in earth gravity because of well-known disruptive instabilities incurred in long-

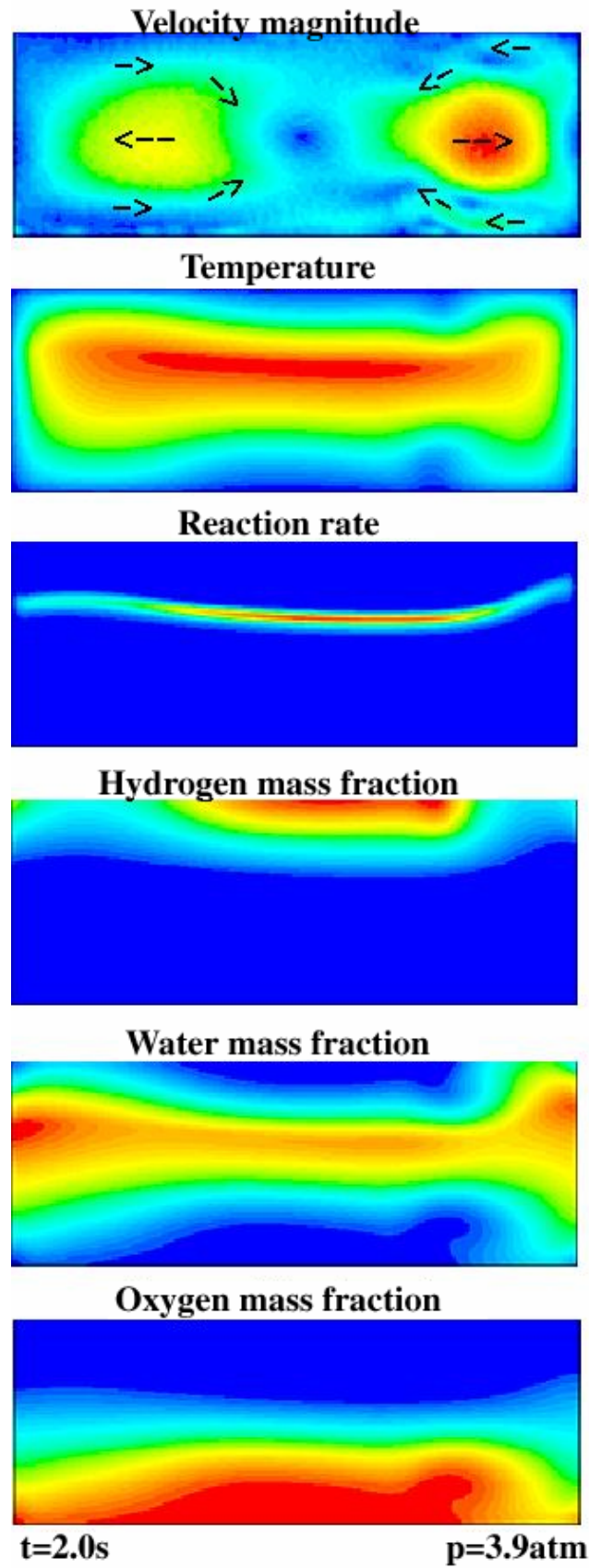


Figure 3b – Flame formation. Velocity, temperature, water production rate, and mass fraction fields 2.0s after separator starts moving at 1m/s. $V_{max}=0.04m/s$, $T_{max}=2446K$, $RR_{max}=0.7Kg/m^3/s$, $[H_2]_{max}=0.0215$, $[H_2O]_{max}=0.2658$, $[O_2]_{max}=0.9727$.

residence counter-flows, would become accessible in microgravity. The practical impact of establishing the plausibility of its success involves the investment of significant resources for the development of a spacecraft apparatus. The arguments to date for viability of the design under discussion are predicated on approximate, subdivisional treatment of phenomena in the container. Such treatments suppress acoustic waves and overlook finite-reaction-rate effects. The technical impact of the numerical treatment presented herein pertains to providing a global solution, with a meticulous treatment of the pressure field in all its 2-D spatial and temporal detail, in an enclosed chamber and with a translating separator.

Initially, a quiescent hydrogen-argon mixture occupies one half-volume, and a oxygen-helium mixture occupies the other half-volume, of a squat rectangular container with impervious, non-catalytic, isothermal walls. A thin separator plate at the centerplane is withdrawn at constant speed, and the flammable mixture formed in its wake by the interpenetration of reactants is ignited near one sidewall. A triple-flame starts to propagate across the centerplane and reaches the other sidewall. Convection is generated during the flame initiation period due to separator motion, triple-flame propagation and flame-induced thermal expansion. Using a container length of 25cm, half-height of 4.5cm, separator-removal speed of 1m/s, and reactant concentrations that correspond to an equivalence ratio of 0.2 if the contents were premixed, the numerical results indicate that the generated convection decays substantially in 2 seconds. During this period, convection enhances the depletion of the stoichiometrically deficient reactant hydrogen and displaces hydrogen near the sidewalls toward the central region of the container.

After 2 seconds, a planar, uniform, diffusion-dominated flame is formed in the central region of the container. The width of the flat flame is about 10cm, and continues to shrink as the reactants diffuse horizontally toward the cold sidewalls, near which quench layers thicken. The pressure in the container rises to about 3.9atm from its initial value of 1atm, and provides further evidence of significant reactant depletion, by comparison with the computed adiabatic, constant-volume value of 6.8atm.

The one and only, but realistic, numerical case studied in this paper suffices to demonstrate that no anomalous phenomena, omitted in the approximate treatments [1–5], significantly alter expectations for the currently existing design and test protocol. Furthermore, the particular case chosen indicates that tests with the fast-diffusing, fast-reacting fuel species H_2 and/or highly "off-stoichiometric" scenarios are suitable for the short microgravity testing time available in some ground-based drop-tower facilities. By inference, space-flight testing is appropriate for stoichiometrically balanced reactants involving hydrocarbon vapors because a longer microgravity testing interval is required.

The conclusions of this study for the initiation of a diffusion flame would not be altered by a parametric study of "stoichiometry", since the triple-flame propagation would be nearly the same along the near-stoichiometric centerplane of the interdiffusion zone. Stoichiometry determines mainly the direction and speed of travel for the established diffusion flame and the associated chamber pressure. In addition, the calculation reveals that it takes about two seconds for convection, induced by the mode of test initiation, to decay under viscous dissipation. This is a significant finding relative to the interval available for useful data collection in a microgravity experimental study of an unsteady diffusion flame.

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13. ABSTRACT (Maximum 200 words) The high degree of spatial symmetry of a planar diffusion flame affords great simplifications for experimental and modeling studies of gaseous fuel combustion. Particularly, in a microgravity environment, where buoyancy effects are negligible, an effectively strain-rate-free, vigorous flame may be obtained. Such a flame can also provide long residence times and large length scales for practical probing of flame structures and soot processes. This 2-D numerical study explores the feasibility of establishing such a planar diffusion flame in an enclosed container utilizing a realistic test protocol for a microgravity experiment. Fuel and oxygen mixtures, initially segregated into two half-volumes of a squat rectangular container by a thin separator, are ignited as soon as a flammable mixture is formed in the wake of the separator withdrawn in the centerplane. A triple-flame ensues that propagates behind the trailing edge of the separator. The results of calculations show that the mechanically- and thermally-induced convection decays in about two seconds. The establishment of a planar diffusion flame after this period seems feasible in the central region of the container with sufficient quantities of reactants left over for subsequent studies. An analysis of the flame initiation and formation process suggests how the feasibility of creating such a flame can be further improved.				
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